Radionuclide Sorption in High-Level Waste Performance Assessment: Abstraction of Results from Experiments and Surface-Complexation Models

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Sorption onto minerals present along groundwater flow paths may help to mitigate radionuclide transport from the potential high-level nuclear waste repository at Yucca Mountain, Nevada. Radionuclide transport models used in probabilistic performance assessment calculations typically use a constant sorption coefficient (K_d) for each radionuclide and each hydrostratigraphic unit. However, constant K_d models do not adequately account for spatial variability in the mineralogy of the adsorbing phases or for variable chemical conditions (i.e., pH, ionic strength, alkalinity, and concentrations of complexing ligands) that may be encountered along groundwater flow paths. In this presentation, alternative approaches are discussed that incorporate aspects of mechanistic sorption models into probabilistic performance assessment calculations. A diffuse-layer surface complexation model is calibrated against laboratory experiments and used to calculate actinide transport parameters. In one approach, parameter distributions are calculated using the diffuse-layer surface complexation model and data on the chemistry of groundwaters from the Yucca Mountain vicinity. Model results are used to provide limits on K_d probability distribution functions as input into performance assessment. Under the groundwater chemical conditions observed in the vicinity of Yucca Mountain, calculated K_ds for some actinides can range over many orders of magnitude. Another approach uses the diffuse-layer surface complexation model to calculate actinide sorption behavior for a wide range of geochemical parameters and to develop response surfaces for actinide sorption (e.g., as functions of pH and pCO₂) for use in performance assessment calculations. These alternative approaches can be adapted readily to current performance assessment abstractions using site-specific information to provide geochemical constraints on radionuclide transport parameters.

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